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It is now generally agreed that the absorption of sound waves in a gas is, in most part, due to the exchange of energy between the sound wave and the translational and internal states of the gas molecules. We develop a theory using the 17-moment approximation[1], from which we are able to calculate the absorption and dispersion of sound in a general polyatomic gas. This theory proves to be general enough to be valid for many internal degrees of freedom, however in our study we consider only rotational and vibrational states.

After much arrangement and manipulation it is possible to obtain a set of linear equations which are of the form of a general eigenvalue-eigenvector equation. Such an equation is convenient to be solved on the computer. We develop computer techniques to solve this eigenvalue-eigenvector equation and, using an IBM 360/75 computer, compute the absorption and dispersion.

It is found that a combination theory arrived at by adding the classical translational and internal absorption compares favorably with our theory for translational and rotational absorption. Considering vibrational absorption as well, we conclude that we are reasonably accurate although we do not find comparison theories.

We observe that the absorption due to internal modes reaches maxima for values of the rarefaction parameter, Λ, approximately equal to one-half the collision number. Our conclusion is that for these values of Λ, the frequency of the wave is in such a relationship with the

collision frequency that maximum amounts of energy can be exchanged between the translational and internal states. It is also observed that for values of Λ much less and much greater than the collision number, the absorption due to the internal states is a minimum. It is our belief that for these collision numbers the collision frequency is in such a mismatch with that of the wave that significant amounts of energy are not able to be exchanged between the internal and translational states.

The dispersion in every case considered proves to be consistently uninteresting. It is observed that the speed of the wave approaches the low frequency limit more slowly as the rotational and/or vibrational collision number(s) is increased.

THE ABSORPTION AND DISPERSION OF SOUND WAVES IN POLYATOMIC GASES

by

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CHAPTER I

INTRODUCTION

In this research we use the 17-moment approximation[1] in the kinetic theory of polyatomic gases to investigate the absorption and dispersion of sound waves in a general polyatomic gas. Our study is limited to polyatomic gases with two and three degrees of freedom respectively, although it can easily be extended to include more internal degrees of freedom. In one case translational and rotational degrees of freedom are investigated whereas in another the two above plus a vibrational degree of freedom are included.

A considerable amount of work has been done in which the absorption and dispersion of sound was investigated. Greenspan[2] considered a simple monatomic gas (a gas with one-atom molecules) in which the only absorption to be considered is the classical translational absorption. Monchick[3] went further to develop a combination theory for a diatomic gas in which not only translational but also internal absorption was considered. This theory, based upon a frequency dependent thermal conductivity, was confined to a range of very low frequencies. On the other hand Hanson and Morse[4] investigated the translational and internal absorption for a diatomic gas in which very high frequencies were considered. Two other workers in the field, Hertzfeld and Litovich[5], looked at just the internal absorption for a diatomic gas. The dispersion of sound, or the gradual change of the speed of sound from the equilibrium

value, was observed by Zel'dovich and Raizer[6] to occur in what is known as the intermediate frequency range. They further noted that the lower speed of sound corresponds to the equilibrium value of the specific heat while the higher speed of sound corresponds to the situation in which the vibrational degree of freedom does not participate in the periodic changes in the state of the gas. In our study a general polyatomic gas is considered which can have many internal degrees of freedom. The dispersion and absorption found from other theories makes an interesting comparison with that due to our theory.

The purpose of the research is to develop computer techniques for solving the set of equations necessary to evaluate the dispersion and absorption of the sound waves. Analytical methods used in solving these equations are impractical. Consequently, the numerical methods we develop using the computer allow us to proceed with not only more speed and accuracy but greater detail. This could not possibly be achieved with analytical calculations.

Arrangement and organization of the thesis is accomplished using several chapters, each one presenting a separate objective. In Chapter II a formal presentation of the mathematical formulations is achieved. Having developed, in Chapter II, the final set of linear equations necessary for determining the absorption and dispersion, a discussion of numerical techniques is brought out in Chapter III. These numerical methods will later be shown to be general enough to solve a set of linear equations for any number of internal degrees of freedom. A discussion and interpretation of results follow in Chapter IV. This chapter is simply a

presentation and explanation of our results in the form of graphs. However it is indeed with caution that we attempt to make generalizations and conclusions, which is the context of Chapter V. Finally in Chapter VI, a brief summary and conclusion of the entire research is presented.

CHAPTER II

MATHEMATICAL FORMULATIONS

In a recent paper, McCormack[7] has derived a closed set of moment equations which are general enough to include gases whose molecules may possess many internal degrees of freedom, and which can be applied to near equilibrium and relaxation type flows. If we focus our attention on McCormack's[7] Eqs. (17), (18), (21), (19), (20), (22), and (23) respectively, and consider motion in the x_1-direction only, then, with N internal modes, the physical properties of interest for the gas are:

n, the particle density;

$\bar{v}_1$, the average velocity of a molecule in the x_1-direction;

P_{11}, the viscous stress;

T_t, the translational temperature;

T_r, the internal temperature for the rth mode;

q_1^t, the translational heat flux;

q_1^r, the internal heat flux for the rth mode;

where r = 1, 2, ..., N.

If we set $x = x_1$, $u = \bar{v}_1$, $P = P_{11}$, $q_t = q_1^t$, $q_r = q_1^r$, and $p = nkT_t$, where k is Boltzman's constant and p is the pressure, then McCormack's[7] Eqs. (17)-(23) can be written in the form

continuity,

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nu) = 0; \tag{1}$$

momentum,

$$mn\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)u + \frac{\partial}{\partial x}(P + p) = 0; \tag{2}$$

viscous stress,

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}\left(u P\right) + \frac{8}{15}\frac{\partial}{\partial x}(q_t) + \frac{4}{3}\left(\mathcal{P}+p\right)\frac{\partial u}{\partial x} = C_1 \; ; \tag{3}$$

translational energy,

$$\frac{3}{2} n k \left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right) T_t + \frac{\partial}{\partial x}(q_t) + \left(\mathcal{P}+p\right)\frac{\partial u}{\partial x} = C_2 \; ; \tag{4}$$

internal energy for the rth mode,

$$n c_r \left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right) T_r + \frac{\partial}{\partial x}(q_r) = C_3^r \; ; \tag{5}$$

translational heat flux,

$$\frac{\partial}{\partial t}(q_t) + \frac{\partial}{\partial x}(u q_t) + \frac{11}{5} q_t \frac{\partial u}{\partial x} + \frac{kT}{m}\frac{\partial P}{\partial x} + \frac{7}{2}\frac{k}{m} P \frac{\partial T}{\partial x}$$

$$- \frac{1}{mn} P \frac{\partial}{\partial x}\left(\mathcal{P}+p\right) + \frac{5}{2}\frac{k}{m} p \frac{\partial T}{\partial x} + \frac{5}{2}\frac{k}{m} P \frac{\partial}{\partial x}\left(T_t - T\right) = C_4 \; ; \tag{6}$$

and internal heat flux for the rth mode,

$$\frac{\partial}{\partial t}(q_r) + \frac{\partial}{\partial x}(u q_r) + q_r \frac{\partial u}{\partial x} + \frac{c_r}{m}\left(\mathcal{P}+p\right)\frac{\partial T}{\partial x}$$

$$+ \frac{c_r}{m} n k T \frac{\partial}{\partial x}\left(T_r - T\right) = C_5^r \; ; \tag{7}$$

where the C's are the inelastic collision integrals defined in Ref. 7, and c_r is the heat capacity per molecule for the rth internal degree of freedom.

McCormack[7] has shown that C_1 and C_2 can be written as

$$C_1 = -\left(n k T_t / \mu\right) \mathcal{P}, \tag{8}$$

$$C_2 = -n \sum_s c_s \left(\frac{T_t - T_s}{\tau_s}\right), \tag{9}$$

where τ_s is the acoustic relaxation time, and μ is the coefficient of viscosity. Using the properties of the collision integrals discussed in Ref. 1, C_3^r can be put in the form

$$C_3^r = -n c_r \left[\frac{T_r - T_t}{\tau_r} + \sum_{s \neq r} \frac{\left(T_r - T_s\right)}{\tau_{rs}}\right], \tag{10}$$

with τ_{rs} being defined as the relaxation time for the temperature equilibration between the rth and sth internal mode.

Monchick[3], neglecting complex collisions, i.e., collisions which alter the state of more than one internal mode of the colliding molecules, has shown that the terms C_4 and C_5 can be written as

$$C_4 = -\frac{2}{3}\left[\frac{nkT}{\mu} + \frac{5}{2k}\sum_s \frac{c_s}{\tau_s}\right] q_t + \frac{5}{6}\sum_s q_s/\tau_s \quad , \tag{11}$$

$$C_5 = \frac{c_r}{3k\tau_r} q_t - \left(\frac{kT}{mD} + \frac{1}{2\tau_r}\right) q_r \quad , \tag{12}$$

where D is the self-diffusion coefficient (assumed the same for each internal mode).

For the purposes of what follow we will find it convenient to define the following dimensionless quantities:

approximate average time between collisions,

$$\tau_{coll} = \frac{\pi\mu}{4p} \quad ;$$

approximate collision frequency,

$$\nu_{coll} = \frac{1}{\tau_{coll}} = \frac{4p}{\pi\mu} \quad ;$$

collision number for the rth mode,

$$Z_r = \frac{\tau_r}{\tau_{coll}} \quad ;$$

"diffusion time",

$$\tau_d = \frac{m n D}{2p} \quad ;$$

"diffusion collision number",

$$Z_d = \frac{\tau_d}{\tau_{coll}} \quad ;$$

and dimensionless specific heat,

$$h_r = \frac{c_r}{k} \cdot$$

Upon substitution of Eqs. (8)-(12) and the dimensionless quantities into Eqs. (1)-(7), we obtain

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nu) = 0 \quad , \tag{13}$$

$$mn\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)u + \frac{\partial}{\partial x}(P+p) = 0 \, , \tag{14}$$

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}(uP) + \frac{8}{15}\frac{\partial}{\partial x}(q_t) + \frac{4}{3}(P+p)\frac{\partial u}{\partial x} = -(nkT_t/\mu)P \quad , \tag{15}$$

$$\frac{3}{2}nk\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)T_t + \frac{\partial}{\partial x}(q_t) + (P+p)\frac{\partial u}{\partial x} = -n\sum_s c_s\frac{(T_t - T_s)}{\tau_s} \, , \tag{16}$$

$$nC_r\left(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x}\right)T_r + \frac{\partial}{\partial x}(q_r) = -nC_r\left[\frac{T_r - T_t}{\tau_r} + \sum_{s\neq r}\frac{(T_r - T_s)}{\tau_{rs}}\right] \, , \tag{17}$$

$$\frac{\partial}{\partial t}(q_t) + \frac{\partial}{\partial x}(uq_t) + \frac{11}{5}q_t\frac{\partial u}{\partial x} + \frac{kT}{m}\frac{\partial P}{\partial x} + \frac{7}{2}\frac{k}{m}P\frac{\partial T}{\partial x}$$

$$-\frac{1}{mn}P\frac{\partial}{\partial x}(P+p) + \frac{5}{2}\frac{k}{m}p\frac{\partial T}{\partial x} + \frac{5}{2}\frac{k}{m}p\frac{\partial}{\partial x}(T_t - T) =$$

$$-\frac{2}{3}\left(\frac{nkT}{\mu} + \frac{5}{6k}\sum_s\frac{c_s}{\tau_s}\right)q_t + \frac{5}{6}\sum_s q_s/\tau_s \, , \tag{18}$$

$$\frac{\partial}{\partial t}(q_r) + \frac{n_r k^2 T}{m}h_r\frac{\partial T_r}{\partial x} = \frac{c_r}{3k\tau_r}q_t - \left(\frac{kT}{m\beta} + \frac{1}{2\tau_r}\right)q_r \, . \tag{19}$$

These equations constitute a closed set of differential equations for the macroscopic properties of the gas. To study the sound problem we assume plane wave solutions of the following form:

$$n = n_0 + n' e^{i(\omega t - \gamma x)} \quad ,$$

$$u = u' e^{i(\omega t - \gamma x)},$$

$$T_t = T_o + T_t' e^{i(\omega t - \gamma x)},$$

$$T_r = T_o + T_r' e^{i(\omega t - \gamma x)} \qquad r = 1, 2, \ldots, N,$$

$$P = P' e^{i(\omega t - \gamma x)},$$

$$q_t = q_t' e^{i(\omega t - \gamma x)},$$

$$q_r = q_r' e^{i(\omega t - \gamma x)} \qquad r = 1, 2, \ldots, N,$$

where ω is the angular frequency; n_o, the ambient density; T_o the ambient temperature; the primed quantities, the departures from the equilibrium values; and

$$\gamma = \omega/c - i\alpha \tag{20}$$

is the wave number, where c is the speed of the wave and α is the absorption coefficient.

If we substitute these assumed solutions into the differential equations, neglect terms quadratic in the departures from equilibrium, and drop the prime notation, we have

$$i\omega n - i\gamma n_o u = 0, \tag{21}$$

$$i\omega m n_o u - i\gamma P - i\gamma k T_o n - i\gamma n_o k T_t = 0, \tag{22}$$

$$i\omega P - i\gamma 8/15\, q_t - i\gamma 4/3\, n_o k T_o u = -n_o/\mu\, k T_o P, \tag{23}$$

$$i\omega 3/2\, n_o k T_t - i\gamma q_t - i\gamma n_o k T_o u = \frac{-4 n_o k p_o}{\pi \mu} \sum_s h_s/Z_s\, (T_t - T_s), \tag{24}$$

$$i\omega n_o k h_r T_r - i\gamma q_r = \frac{-4 n_o k p_o}{\pi \mu}\, h_r/Z_r\, (T_r - T_t), \tag{25}$$

$$i\omega q_t - i\gamma k T_o P/m - i\gamma 5 n_o k^2 T_o T_t/2m$$

$$= -2/3 \left(\frac{P_o}{\mu} + \frac{10}{3\pi}\frac{P_o}{\mu} \sum_s \frac{h_s}{Z_s}\right) q_t + \frac{10}{3\pi}\frac{P_o}{\mu} \sum_s \frac{q_s}{Z_s}, \tag{26}$$

$$i\omega q_r - i\gamma n_o k^2 T_o h_r T_r/m = \frac{4p_o h_r}{3\pi\mu Z_r} q_t - \frac{2p_o}{\pi\mu}(1/Z_d + 1/Z_r)q_r, \qquad (27)$$

where $p_o = n_o k T_o$ is the ambient pressure. In terms of the rarefaction parameter, $\Pi = p_o/\mu\omega$, (which is approximately the ratio of the collision frequency to the sound frequency) and the adiabatic sound speed $c_o = (\gamma_o kT_o/m)^{\frac{1}{2}}$, where γ_o is the ratio of the specific heat at constant pressure to the specific heat at constant volume, and T_o is the ambient temperature, we can write Eqs. (21)-(27) in dimensionless form as

$$\lambda X_1 - X_2 = 0, \qquad (28)$$

$$\lambda X_2 - X_3 - \frac{1}{\gamma_o} X_1 - \frac{1}{\gamma_o} X_4 = 0, \qquad (29)$$

$$\lambda(1-i\Pi)X_3 - 8/15\ X_5 - \frac{1}{\gamma_o} 4/3\ X_2 = 0, \qquad (30)$$

$$\lambda(3/2-i4a\frac{\Pi}{\pi})\frac{1}{\gamma_o} X_4 - X_5 - \frac{1}{\gamma_o} X_2 + \frac{\lambda\Pi i4}{\pi\gamma_o}\sum_{r=1}^{N} h_r/Z_r\ Y_r = 0, \qquad (31)$$

$$\lambda(1-\frac{i4}{Z_1}\frac{\Pi}{\pi})\frac{1}{\gamma_o} h_r Y_r - Y_r' + \frac{\lambda\Pi}{\pi\gamma_o} i4h_r/Z_r\ X_4 = 0, \qquad (32)$$

$$\lambda(1-\frac{i2}{3}\Pi(1+10a/(3\pi)))X_5 - \frac{1}{\gamma_o} X_3 - 5X_4/(2\gamma_o^2) + \frac{\lambda\Pi}{3\pi} i10\sum_{r=1}^{N}\frac{Y_r'}{Z_r} = 0, \qquad (33)$$

$$\lambda(1-\frac{\Pi}{\pi} i2(1/Z_d+1/Z_r))Y_r' + \frac{1}{\gamma_o^2} h_r Y_r + \frac{\lambda\Pi}{3\pi} i4h_r/Z_r\ X_5 = 0, \qquad (34)$$

with r = 1, 2, ..., N and where

$$X_1 = n/n_o,\ X_2 = u/c_o,\ X_3 = P/(n_o mc_o^2),\ X_4 = T_t/T_o,$$

$$X_5 = q_t/(mn_o c_o^3),\ Y_r = T_r/T_o,\ Y_r' = q_r/(mn_o c_o^3),\ a = \sum_s \frac{h_s}{Z_s},$$

and

$$\lambda = \omega/c_o\gamma\ . \qquad (35)$$

As mentioned earlier, we want to investigate the case where we have just one internal mode and later on the case with two internal

modes. If we restrict our attention now to the first case (corresponding to N = 1) and make the following definitions:

$$X_6 = Y_1 = T_{int}/T_o, \quad X_7 = Y_1' = q_{int}/(mn_o c_o^3),$$

$$\beta_1 = (1 - \tfrac{\Pi}{\pi} i2(1/Z_d + 1/Z_1)), \quad \delta_1 = (1 - \tfrac{\Pi}{\pi} i4/Z_1),$$

$$\theta_1 = (1 - i2/3\Pi(1+10a/(3\pi))), \quad \theta_2 = (3/2 - \tfrac{\Pi}{\pi} i4a),$$

$$\omega_1 = (1 - i\Pi),$$

we can write Eqs. (28)-(34) as

$$X_2 = \lambda X_1, \tag{36}$$

$$\tfrac{1}{\gamma_o} X_1 + X_3 + \tfrac{1}{\gamma_o} X_4 = \lambda X_2, \tag{37}$$

$$\tfrac{1}{\gamma_o} \frac{4X_2}{3} + \frac{8X_5}{15} = \lambda \omega_1 X_3, \tag{38}$$

$$\tfrac{1}{\gamma_o} X_2 + X_5 = \tfrac{\lambda}{\gamma_o} \theta_2 X_4 + \tfrac{\lambda \Pi}{\pi \gamma_o} i4h_1/Z_1 X_6, \tag{39}$$

$$X_7 = \tfrac{\lambda \Pi}{\pi \gamma_o} i4h_1/Z_1 \; X_4 + \tfrac{\lambda \delta_1}{\gamma_o} h_1 X_6, \tag{40}$$

$$\tfrac{1}{\gamma_o} X_3 + \tfrac{1}{\gamma_o^3} 5/2 \; X_4 = \lambda \theta_1 X_5 + \tfrac{\lambda \Pi}{\pi} i10/(3Z_1) \; X_7, \tag{41}$$

$$\tfrac{1}{\gamma_o^3} h_1 X_6 = \tfrac{\lambda \Pi}{\pi} i4h_1/(3Z_1) \; X_5 + \lambda \beta_1 X_7. \tag{42}$$

Equations (36)-(42) constitute a set of seven linear equations in seven unknowns and are of the form of the general eigenvalue-eigenvector equation, viz.,

$$A \vec{X} = \lambda B \vec{X}, \tag{43}$$

where λ is the eigenvalue, $\vec{X}$, the eigenvector given by

$$\vec{X} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \end{bmatrix},$$

and where A and B are the matrices of the coefficients which have the values

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\gamma_\infty} & 0 & 1 & \frac{1}{\gamma_\infty} & 0 & 0 & 0 \\ 0 & 4/(3\gamma_\infty) & 0 & 0 & 8/15 & 0 & 0 \\ 0 & \frac{1}{\gamma_\infty} & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & \frac{1}{\gamma_\infty} & 5/(2\gamma_\infty^2) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_1/\gamma_\infty^2 & 0 \end{bmatrix},$$

and

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \omega_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \theta_2/\gamma_\infty & 0 & \frac{i4h_1\Pi}{Z_1\pi\gamma_\infty} & 0 \\ 0 & 0 & 0 & \frac{i4h_1\Pi}{Z_1\pi\gamma_\infty} & 0 & \delta_1 h_1/\gamma_\infty & 0 \\ 0 & 0 & 0 & 0 & \theta_1 & 0 & \frac{i10\Pi}{3Z_1\pi} \\ 0 & 0 & 0 & 0 & \frac{i4h_1\Pi}{3Z_1\pi} & 0 & \beta_1 \end{bmatrix}.$$

As can easily be seen, it would be a horrendous task to solve the equations analytically, so we therefore rely upon the computer and numerical methods. What is sought is the solution of the equations for the λ's and X's. From the λ's we can determine the absorption and dispersion of the sound wave and from the X's we can evaluate the dimensionless quantities defined previously as $X_1, X_2, \ldots, X_7$.

CHAPTER III

PROGRAMMING CONSIDERATIONS

Referring to Eq. (43) we observe that A and B are both complex matrices with no special symmetry properties. If Eq. (43) is multiplied by the inverse of B, we obtain

$$B^{-1}A\vec{X} = \lambda B^{-1}B\vec{X} \ ,$$

or

$$A'\vec{X} = \lambda\vec{X} \ , \tag{44}$$

where $A' = B^{-1}A$, and is likewise complex.

One approach to the problem of calculating the eigenvalues and eigenvectors of a complex matrix has been given by Ralston[8]. The technique involves writing a complex matrix, A, in terms of its real and imaginary parts such as

$$A = B + iC.$$

Ralston[8] then shows that an eigenvalue of A is also an eigenvalue of

$$D = \begin{bmatrix} B & -C \\ C & B \end{bmatrix} ,$$

where the order of D is twice that of A.

Available in the IBM PL/1 scientific subroutine library are subroutines for finding the eigenvalues and eigenvectors of a general n x n real nonsymmetric matrix, the eigenvalues and eigenvectors themselves in general being complex. The programming problem therefore reduces to writing a driving program to call on the subroutines MATE, MEAT, MVAT, and MVEB[9] which compute the eigenvalues and eigenvectors and then format

the output according to our specifications. Subroutine MATE reduces a real matrix to Hessenberg form using elimination techniques. Control then passes to subroutine MEAT which computes the eigenvalues of the Hessenberg matrix using double QR iteration. After this is done, subroutine MVAT is called to obtain the eigenvectors of the Hessenberg matrix. Finally subroutine MVEB gives the eigenvectors corresponding to our original matrix using back transformation and elimination techniques.

It is felt that a brief discussion of the function of the overall program will be of benefit as an explanation to our technique, and later, to some problems encountered. The input parameters to the program are the dimensions of the complex matrix, the dimensionless specific heat, h_r, the diffusion collision number, Z_d, and the internal collision number, Z_r. It should be emphasized that the program is general enough to handle any number of internal degrees of freedom. After obtaining the input data, the program generates the elements of both the A and B matrices. This step of the program is necessarily preceeded by the input data since the elements of the matrices depend upon these parameters. The B matrix is fed into subroutine MATINV, written by McCormack[10], which computes the inverse of B. Matrix A is multiplied by the inverse of B to obtain the matrix A' whose eigenvalues and eigenvectors we seek. The A' matrix is then expanded into a real matrix of double the order. This matrix is in turn fed into the four subroutines for computing the eigenvalues and eigenvectors.

Since the expanded matrix is double the order of A', we are really interested in only half the number of eigenvalues and eigenvectors computed. Therefore a check is made to determine if each eigenvalue and

corresponding eigenvector of the expanded matrix also satisfy Eq. (44). If we find a true pair then we can compute the dispersion and absorption of the sound wave for particular values of the parameters. We note from Eqs. (20) and (35) that the reciprocal of the eigenvalue is

$$\frac{1}{\lambda} = \frac{c_o}{c} - i\alpha c_o/\omega \ ,$$

where the real part of $1/\lambda$ is the dispersion, c_o/c, and the negative imaginary part is the absorption, $\frac{\alpha}{\omega} c_o$. Physically the dispersion refers to the degree to which the speed of the wave deviates from the adiabatic value, c_o, and the absorption refers to the amount by which the amplitude of the wave is changed. The remainder of the program formats the output as follows: λ , the eigenvalue; Z_r, the internal collision number; $(c-c_o)/c_o$, the ratio of the speeds; the components of the eigenvectors; the angular separation of each component of the eigenvector relative to the first component, X_1; and the magnitude of each component relative to the first.

The number of eigenvalues and eigenvectors of the matrix A' is, of course, equal to the dimensions of the matrix. Upon examination of all the eigenvalues and eigenvectors, we conclude that only one is of physical interest. The others correspond to either the case of a wave which is attenuated so rapidly that it cannot be measured or to a wave which has a negative absorption coefficient which implies the physically meaningless situation in which the wave is amplified by the gas.

If the procedures outlined above are carried out it is found that the subroutines MATE, MEAT, MVAT, and MVEB which, it is claimed, are capable of handling a general matrix, do not work properly for our matrix, A'.

This is the problem alluded to earlier. The only reason we can determine for this failure is that the subroutines were not written to handle a matrix such as A' which has all zeros on the diagonal.

We found that we could circumvent this difficulty by analytically reducing Eqs. (36)-(42) to a system of three equations through elimination of X_2, X_3, X_5, and X_7. The system, involving X_1, X_4, and X_6 is given by

$$\frac{1}{\gamma_*}X_1 + \frac{8}{15\omega_1\gamma_*}\Theta_2 X_4 + \frac{24}{30\omega_1\gamma_*}X_1 + \frac{32}{15}\frac{ih_1\pi}{Z_1\omega_1\pi\gamma_*}X_6 + \frac{1}{\gamma_*}X_4 = \lambda^2 X_1, \quad (45)$$

$$\frac{8\Theta_2}{15\omega_1\gamma_*^2}X_4 + \frac{24}{30\omega_1\gamma_*^2}X_1 + \frac{32}{15}\frac{ih_1\pi}{Z_1\omega_1\pi\gamma_*^2}X_6 + \frac{5}{2\gamma_*^2}X_4 = -\frac{5\Theta_1\lambda^2}{2\gamma_*}X_1$$
$$+ \Theta_1\Theta_2\frac{\lambda^2}{\gamma_*}X_4 + \frac{3\Theta_1\lambda^2}{2\gamma_*}X_1 + \frac{4ih_1\Theta_1\pi\lambda^2}{Z_1\pi\gamma_*}X_6 - \frac{40h_1\pi^2\lambda^2}{3Z_1^2\pi^2\gamma_*}X_4$$
$$+ \frac{10ih_1\pi\delta_1\lambda^2}{3Z_1\pi\gamma_*}X_6, \quad (46)$$

$$\frac{1}{\gamma_*^2}h_1 X_6 = -\frac{10ih_1\pi\lambda^2}{3Z_1\pi\gamma_*}X_1 + \frac{4ih_1\Theta_2\pi\lambda^2}{3Z_1\pi\gamma_*}X_4 + \frac{2ih_1\pi\lambda^2}{Z_1\pi\gamma_*}X_1$$
$$- \frac{16h_1^2\pi^2\lambda^2}{3Z_1^2\pi^2}X_6 + \frac{4ih_1\pi\beta_1\lambda^2}{Z_1\pi\gamma_*}X_4 + \frac{\beta_1\delta_1\lambda^2}{\gamma_*}h_1 X_6, \quad (47)$$

which is of the form of Eq. (43), where now the eigenvalue is λ^2 and A and B are given by

$$A = \begin{bmatrix} \left(\frac{1}{\gamma_*} + \frac{4}{5\omega_1\gamma_*}\right) & \left(\frac{1}{\gamma_*} + \frac{8\Theta_2}{15\omega_1\gamma_*}\right) & \frac{32ih_1\pi}{15Z_1\omega_1\pi\gamma_*} \\ \frac{4}{5\omega_1\gamma_*^2} & \left(\frac{5}{2\gamma_*^2} + \frac{8\Theta_2}{15\omega_1\gamma_*^2}\right) & \frac{32ih_1\pi}{15Z_1\omega_1\pi\gamma_*^2} \\ 0 & 0 & \frac{h_1}{\gamma_*^2} \end{bmatrix},$$

$$B = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{\Theta_1}{\gamma_0} & \left(\frac{\Theta_1\Theta_2}{\gamma_0} - \frac{40h_1}{3Z_1^2}\frac{\Pi^2}{\pi^2\gamma_0}\right) & \frac{ih_1}{Z_1}\frac{\Pi}{\pi}\left(\frac{4\Theta_1}{\gamma_0} + \frac{10}{3}\frac{\delta_1}{\gamma_0}\right) \\ -\frac{i4h_1}{3Z_1}\frac{\Pi}{\pi\gamma_0} & \frac{ih_1}{Z_1}\frac{\Pi}{\pi}\left(\frac{4\beta_1}{\gamma_0} + \frac{4\Theta_2}{3\gamma_0}\right) & \left(\frac{h_1\beta_1\delta_1}{\gamma_0} - \frac{16h_1^2\Pi^2}{3Z_1^2\pi^2\gamma_0}\right) \end{bmatrix}.$$

To handle the reduced matrices, the program is changed only slightly in that now we no longer take the reciprocal of λ but the reciprocal square root, since the equations are in terms of λ^2. Also, the X_2, X_3, X_5, and X_7 components of each eigenvector are not computed explicitly but are given in terms of X_1, X_4, and X_6 by

$$X_2 = \lambda X_1,$$

$$X_3 = \frac{8\Theta_2}{15}\frac{1}{\omega_1\gamma_0}X_4 + \frac{24}{30}\frac{1}{\omega_1\gamma_0}X_1 + \frac{32ih_1}{15Z_1}\frac{\Pi}{\omega_1\pi\gamma_0}X_6,$$

$$X_5 = \frac{15}{8}\lambda\omega_1 X_3 - \frac{5}{2}\frac{\lambda}{\gamma_0}X_1,$$

$$X_7 = \frac{h_1\delta_1\lambda}{\gamma_0}X_6 + \frac{i4h_1\Pi\lambda}{Z_1\pi\gamma_0}X_4.$$

Upon making these slight changes in the input matrices and the program itself, it is found that the subroutines function properly. The results are discussed in Chapter IV.

If we go back to Eqs. (28)-(34) and consider the case for two internal modes (corresponding to N = 2) we can write

$$X_2 = \lambda X_1, \tag{48}$$

$$\frac{1}{\gamma_0}X_1 + X_3 + \frac{1}{\gamma_0}X_4 = \lambda X_2, \tag{49}$$

$$\frac{4}{3\gamma_0}X_2 + \frac{8}{15}X_5 = \lambda\omega_1 X_3, \tag{50}$$

$$\frac{1}{\gamma_0} X_2 + X_5 = \frac{\Theta_2 \lambda}{\gamma_0} X_4 + \frac{i4h_1 \pi \lambda}{Z_1 \pi \gamma_0} X_6 + \frac{i4h_2 \pi \lambda}{Z_2 \pi \gamma_0} X_7, \tag{51}$$

$$X_8 = \frac{i4h_1 \pi \lambda}{Z_1 \pi \gamma_0} X_4 + \frac{h_1 \delta_1 \lambda}{\gamma_0} X_6, \tag{52}$$

$$X_9 = \frac{i4h_2 \pi \lambda}{Z_2 \pi \gamma_0} X_4 + \frac{h_2 \delta_2 \lambda}{\gamma_0} X_7, \tag{53}$$

$$\frac{1}{\gamma_0} X_3 + \frac{5}{2} \frac{1}{\gamma_0^2} X_4 = \lambda \Theta_1 X_5 + \frac{i10\pi\lambda}{3Z_1 \pi} X_8 + \frac{i10\pi\lambda}{3Z_2 \pi} X_9, \tag{54}$$

$$\frac{1}{\gamma_0^2} h_1 X_6 = \frac{i4h_1 \pi \lambda}{3Z_1 \pi} X_5 + \lambda \beta_1 X_8, \tag{55}$$

$$\frac{1}{\gamma_0^2} h_2 X_7 = \frac{i4h_2 \pi \lambda}{3Z_2 \pi} X_5 + \lambda \beta_2 X_9, \tag{56}$$

where

$$\beta_2 = (1 - \frac{i2\pi}{\pi} (1/Z_d + 1/Z_2)),$$

$$\delta_2 = (1 - \frac{i4\pi}{Z_2 \pi}),$$

$$X_6 = Y_1, \; X_7 = Y_2, \; X_8 = Y_1', \; X_9 = Y_2' .$$

The number of equations are again reduced for programming purposes, by eliminating X_2, X_3, X_5, X_8, and X_9 from Eqs. (48)-(56). We then obtain

$$\frac{1}{\gamma_0} X_1 + \frac{8\Theta_2}{15\omega_1 \gamma_0} X_4 + \frac{24}{30\omega_1 \gamma_0} X_1 + \frac{i32h_1\pi}{15Z_1\omega_1\pi\gamma_0} X_6 + \frac{i32h_2\pi}{15Z_2\omega_1\pi\gamma_0} X_7 + \frac{1}{\gamma_0} X_4 = \lambda^2 X_1, \tag{57}$$

$$\frac{4}{5\omega_1\gamma_0^2} X_1 + \frac{8\Theta_2}{15\omega_1\gamma_0^2} X_4 + \frac{i32h_1\pi}{15Z_1\omega_1\pi\gamma_0^2} X_6 + \frac{i32h_2\pi}{15Z_2\omega_1\pi\gamma_0^2} X_7 + \frac{5}{2\gamma_0^2} X_4 =$$

$$- \frac{\Theta_1 \lambda^2}{\gamma_0} X_1 + \frac{\Theta_1 \Theta_2 \lambda^2}{\gamma_0} X_4 - \frac{40\pi^2}{3\gamma_0\pi^2} \left(\frac{h_1}{Z_1^2} + \frac{h_2}{Z_2^2} \right) \lambda^2 X_4 +$$

$$\frac{ih_1\pi}{Z_1\pi} \left(\frac{10\delta_1}{3\gamma_0} + \frac{4\Theta_1}{\gamma_0} \right) \lambda^2 X_6 + \frac{ih_2\pi}{Z_2\pi} \left(\frac{10\delta_2}{3\gamma_0} + \frac{4\Theta_1}{\gamma_0} \right) \lambda^2 X_7, \tag{58}$$

$$\frac{1}{\gamma_0^2} h_1 X_6 = - \frac{i4h_1\pi\lambda^2}{3Z_1\pi\gamma_0} X_1 + \frac{ih_1\pi}{Z_1\pi} \left(\frac{4\beta_1}{\gamma_0} + \frac{4\Theta_2}{3\gamma_0} \right) \lambda^2 X_4$$

$$+ \left(\frac{h_1 \beta_1 \delta_1}{\gamma_0} - \frac{16 h_1^2 \pi^2}{3 Z_1^2 \pi^2 \gamma_0} \right) \lambda^2 X_6 - \frac{16 h_1 h_2 \pi^2}{3 Z_1 Z_2 \pi^2 \gamma_0} \lambda^2 X_7, \tag{59}$$

$$\frac{1}{\gamma_0^2} h_1 X_7 = - \frac{4 h_2 \pi}{3 Z_2 \pi \gamma_0} \lambda^2 X_1 + \frac{i h_2 \pi}{Z_2 \pi} \left(\frac{4 \beta_2}{\gamma_0} + \frac{4 \theta_2}{3 \gamma_0} \right) \lambda^2 X_4$$

$$- \frac{16 h_1 h_2 \pi^2}{3 Z_1 Z_2 \pi^2 \gamma_0} \lambda^2 X_6 + \left(\frac{h_2 \beta_2 \delta_2}{\gamma_0} - \frac{16 h_2^2 \pi^2}{3 Z_2^2 \pi^2 \gamma_0} \right) \lambda^2 X_7, \tag{60}$$

with

$$X_2 = \lambda X_1,$$

$$X_3 = \frac{8 \theta_2}{15 \omega_1 \gamma_0} X_4 + \frac{24}{30 \omega_1 \gamma_0} X_1 + \frac{i 32 h_1 \pi}{15 Z_1 \omega_1 \pi \gamma_0} X_6 + \frac{i 32 h_2 \pi}{15 Z_2 \omega_1 \pi \gamma_0} X_7,$$

$$X_5 = \frac{15 \lambda \omega_1}{8} X_3 - \frac{5}{2 \gamma_0} \lambda X_1,$$

$$X_8 = \frac{h_1 \lambda \delta_1}{\gamma_0} X_6 + \frac{i 4 h_1 \lambda \pi}{Z_1 \pi \delta_0} X_4,$$

$$X_9 = \frac{h_2 \lambda \delta_2}{\gamma_0} X_7 + \frac{i 4 h_2 \lambda \pi}{Z_2 \pi \gamma_0} X_4 .$$

Eqs. (57)-(60) are again of the form of Eq. (43) where

$$A = \begin{bmatrix} \left(\frac{1}{\gamma_0} + \frac{4}{5 \omega_1 \gamma_0} \right) & \left(\frac{1}{\gamma_0} + \frac{8 \theta_2}{15 \omega_1 \gamma_0} \right) & \frac{i 32 h_1 \pi}{15 Z_1 \omega_1 \pi \gamma_0} & \frac{i 32 h_2 \pi}{15 Z_2 \omega_1 \pi \gamma_0} \\ \frac{4}{5 \omega_1 \gamma_0^2} & \left(\frac{5}{2 \gamma_0^2} + \frac{8 \theta_2}{15 \omega_1 \gamma_0^2} \right) & \frac{i 32 h_1 \pi}{15 Z_1 \omega_1 \pi \gamma_0^2} & \frac{i 32 h_2 \pi}{15 Z_2 \omega_1 \pi \gamma_0^2} \\ 0 & 0 & \frac{h_1}{\gamma_0^2} & 0 \\ 0 & 0 & 0 & \frac{h_2}{\gamma_0^2} \end{bmatrix},$$

$$\vec{X} = \begin{bmatrix} X_1 \\ X_4 \\ X_6 \\ X_7 \end{bmatrix},$$

and

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{\Theta_1}{\gamma_0} & \frac{\Theta_1\Theta_2}{\gamma_0} - \frac{40\pi^2}{3\pi^3\gamma_0}\left(\frac{h_1}{Z_1^2} + \frac{h_2}{Z_2^2}\right) & \frac{ih_1\pi}{Z_1\pi}\left(\frac{4\Theta_1}{\gamma_0} + \frac{10\delta_1}{3\gamma_0}\right) & \frac{ih_2\pi}{Z_2\pi}\left(\frac{10\delta_2}{3\gamma_0} + \frac{4\Theta_1}{\gamma_0}\right) \\ -\frac{i4h_1\pi}{3Z_1\pi\gamma_0} & \frac{ih_1\pi}{Z_1\pi}\left(\frac{4\beta_1}{\gamma_0} + \frac{4\Theta_2}{3\gamma_0}\right) & \left(\frac{h_1\beta_1\delta_1}{\gamma_0} - \frac{16h_1^2\pi^2}{3Z_1^2\pi^2\gamma_0}\right) & -\frac{16h_1h_2\pi^2}{3Z_1Z_2\pi^2\gamma_0} \\ -\frac{i4h_2\pi}{3Z_2\pi\gamma_0} & \frac{ih_2\pi}{Z_2\pi}\left(\frac{4\beta_2}{\gamma_0} + \frac{4\Theta_2}{3\gamma_0}\right) & -\frac{16h_1h_2\pi^2}{3Z_1Z_2\pi^2\gamma_0} & \left(\frac{h_2\beta_2\delta_2}{\gamma_0} - \frac{16h_2^2\pi^2}{3Z_2^2\pi^2\gamma_0}\right) \end{bmatrix}.$$

With but few changes the computer program works with these matrices and calculates absorption and dispersion for two internal degrees of free- in the same manner as indicated in the N = 1 case.

We find it informative now to amend the program somewhat, for the N = 1 case only, such that, in addition to calculating the absorption and dispersion for our theory, it calculates, for comparison purposes, the absorption and dispersion due to the classical translational and internal modes. These comparison criteria later serve to validate our results.

The mathematical expressions for the classical and internal absorption and dispersion can be obtained using the results of Zel'dovich and Raizer[6], Greenspan[2], and Mason and Monchick[11]. Let us represent the internal absorption and dispersion by a quantity χ_r defined by

$$\chi_r = (c_o/c)_r - i(\alpha c_o/\omega)_r,$$

where as before, the real part of χ_r is the dispersion and the negative of the imaginary part of χ_r is the absorption. With the aid of work of Zel'dovich and Raizer[6], it can be shown that

$$\chi_r = \left[\gamma_0 \cdot \frac{3/2 + \dfrac{h_1}{(1 + i\pi Z_1/(4\pi))}}{5/2 + \dfrac{h_1}{(1 + i\pi Z_1/(4\pi))}}\right]^{\frac{1}{2}}. \qquad (61)$$

The classical translational absorption and dispersion is obtained in the following manner. As Greenspan[2] does, we introduce a quantity s defined by

$$\frac{\pi}{s} = f \frac{k}{c_r},$$

where f is the Euken factor given by Mason and Monchick[11] as

$$f = \frac{3}{2} f_{tr} + h_1 f_{int},$$

with

$$f_{tr} = \frac{5}{2}\left(- \frac{10h_1}{3Z_1\pi}\left(1 - \frac{Z_d\pi}{5}\right)\right),$$

and

$$f_{int} = \frac{Z_d\pi}{2}\left(1 + \frac{5}{Z_1\pi}\left(1 - \frac{Z_d\pi}{5}\right)\right).$$

If we choose χ_c to represent the classical translational absorption and dispersion, i.e., $\chi_c = (c_o/c)_c - i(\alpha c/\omega)_c$, then in terms of the above

$$\chi_c^2 = \frac{s\gamma_o}{2} \frac{\gamma_o + i\left(\frac{1}{s} + \frac{4}{3\pi}\right) \pm \left(\left(\gamma_o + i\left(\frac{1}{s} + \frac{4}{3\pi}\right)\right)^2 - \frac{4}{s}\left(i - \frac{4}{3\pi}\right)\right)^{\frac{1}{2}}}{(i - 4\pi/3)}.$$

When computing values of χ_c, the negative square root is taken because the positive square root does not correspond to a traveling wave.

Recalling that for the N = 1 case our theory represents the combined effect of translational and internal absorption and dispersion, it is found that a convenient means of comparison is to algebraically add the separate expressions for the classical translational and internal absorption and dispersion. What is done then is to compare the sum with our theory and observe if indeed the sum theory is valid.

A discussion together with an interpretation and comparison of results follows. The solutions for the translational and internal effects separately are compared to our theory for combined absorption.

CHAPTER IV

DISCUSSION AND INTERPRETATION OF RESULTS

In the following discussion we wish to first consider the N = 1 case and compare the sum of the internal and classical theories with our theory for the absorption. Later on we discuss the N = 2 case but without a comparison theory, having deduced that if we are accurate for N = 1, the N = 2 case must also be valid.

All graphs will be plots of the absorption and dispersion versus Π, the rarefaction parameter. At the very top of each graph will be the dispersion curve for our theory only. Recall that $\Pi = p_o/\mu\omega$ where ω is the angular frequency. Consequently small values of Π correspond to high frequencies, and vice versa. It should also be recalled that Z_1 is the number of collisions necessary for the rotational and translational states to come to equilibrium after having been disturbed by a wave front passing through the gas. In other words, Z_1 is the number of collisions necessary for the temperature and average energy of the rotational state to become the same as that of the translational state. We do not at any time propose that there are any gases existing with our assumed collision numbers; however if one does exist then we have reason to assume it will behave as our theory predicts.

In Fig. 1 is plotted the case for N = 1, Z_1 = 1. The dispersion (c_o/c) curve, starts out at about 0.56, is fairly constant from Π = 0.1 to 0.5, rises gradually from a value of 0.63 at Π = 0.5 to 0.98 for Π = 10, and is asymptotic to 1 for larger Π. As $c_o/c \rightarrow 1$ then $c \rightarrow c_o$ and the

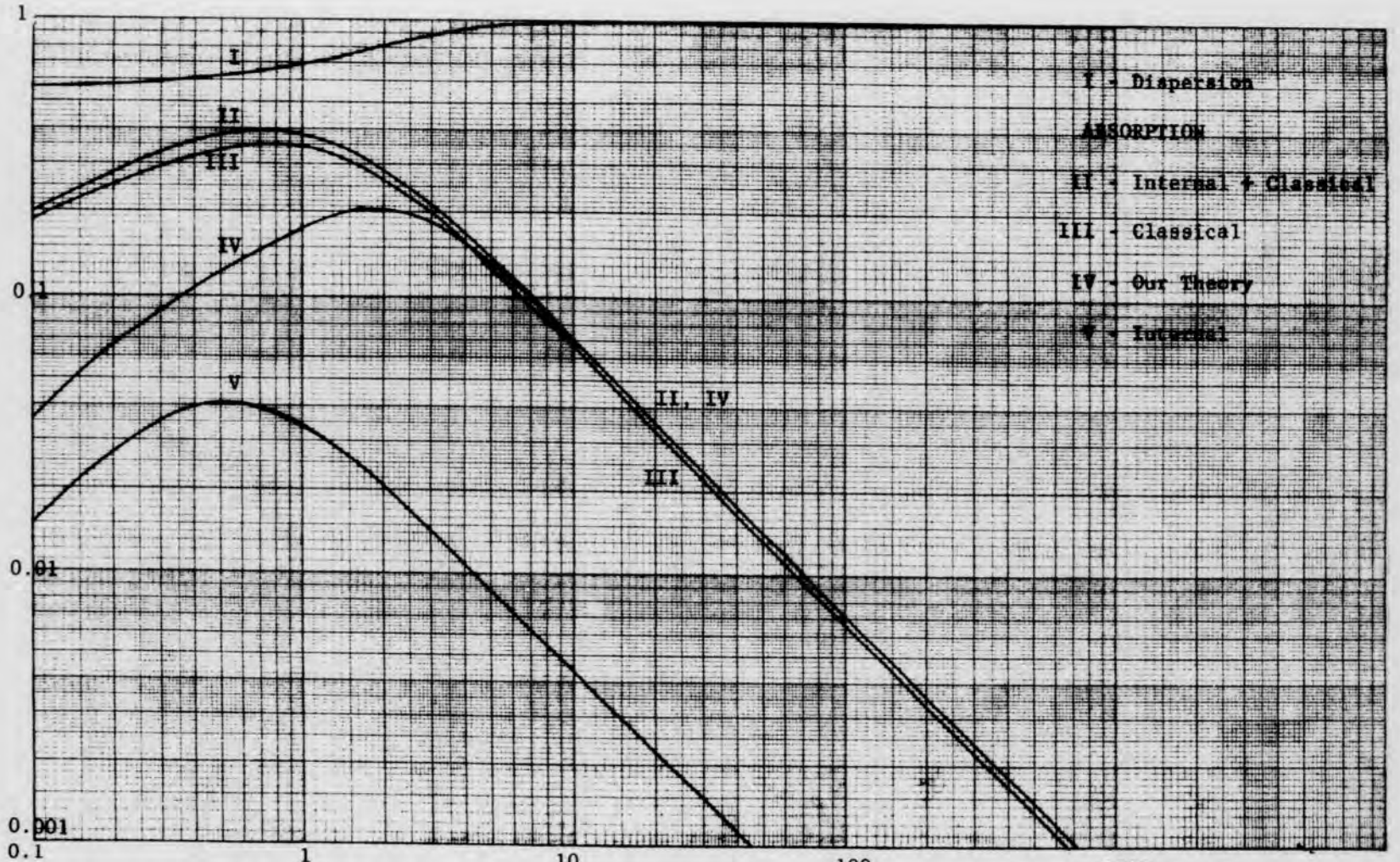

Figure 1. Dispersion and absorption versus the rarefaction parameter for N = 1, h_1 = 1, Z_1 = 1, Z_d = 1

speed of the wave approaches its low frequency limit (c_o). The classical absorption curve is plotted in Fig. 1 but not in the other figures, since it does not change shape for any variation in our parameters. The internal absorption curve is plotted for every N = 1 case. Although it does not change shape, it is translated to the right as Z_1 is increased. In Fig. 1 this curve peaks out close to but less than a value of π equal to 0.5. One can see that the curve representing the sum of the internal and the classical absorption, hereinafter referred to as the sum curve, differs little from the classical curve, the largest difference being near $\pi = 0.5$. Our theory shows less absorption for $\pi < 10$ but for $\pi > 10$ coincides with the sum curve.

For N = 1 and $Z_1 = 10$, as shown in Fig. 2, the dispersion curve starts off again near 0.56 but rises more gradually, and reaches a value of 0.98 near $\pi = 20$. The internal absorption curve is shifted to the right, so that it peaks out near $\pi = 5$. Consequently the deviation of the sum curve from the classical curve is greatest near $\pi = 5$, as seen by the very slight inflection in the curve at that point. Our theory indicates this same inflection near $\pi = 5$. The curve for our theory is less than the sum curve for $\pi < 20$ but coincides with it for $\pi > 20$.

Some interesting results are obtained for Z_1 even larger. For N = 1 and $Z_1 = 100$ (Fig. 3) the internal absorption curve is shifted so that it reaches a maximum near $\pi = 50$. Therefore when the internal absorption curve is added to the classical curve, there is a noticeable flattening in the sum curve near this value of π. It is indeed not a secondary peak since as π is increased $\propto c_o/\omega$ does not increase but only

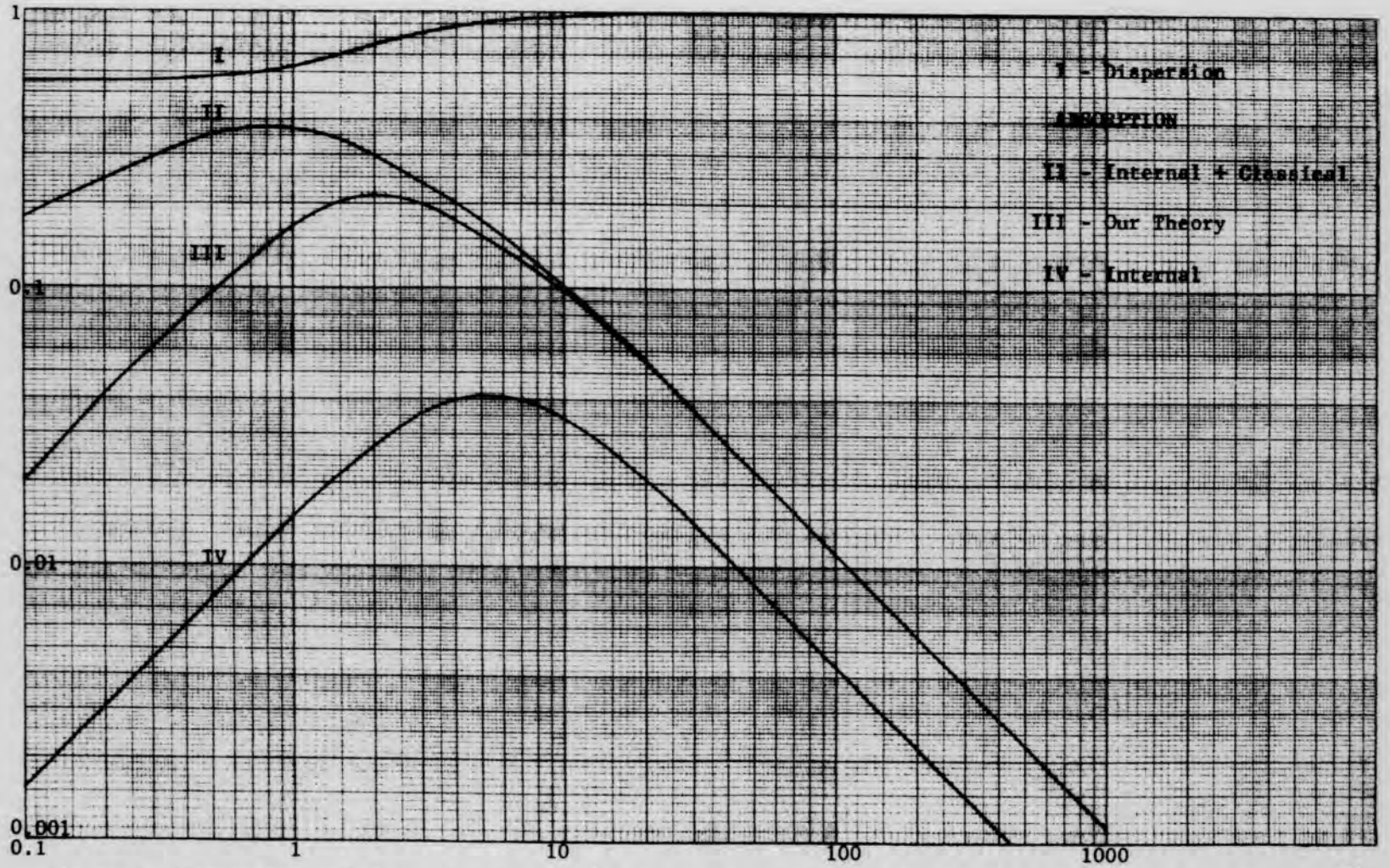

Figure 2. Dispersion and absorption versus the rarefaction parameter for N = 1, h_1 = 1, Z_1 = 10, Z_d = 1

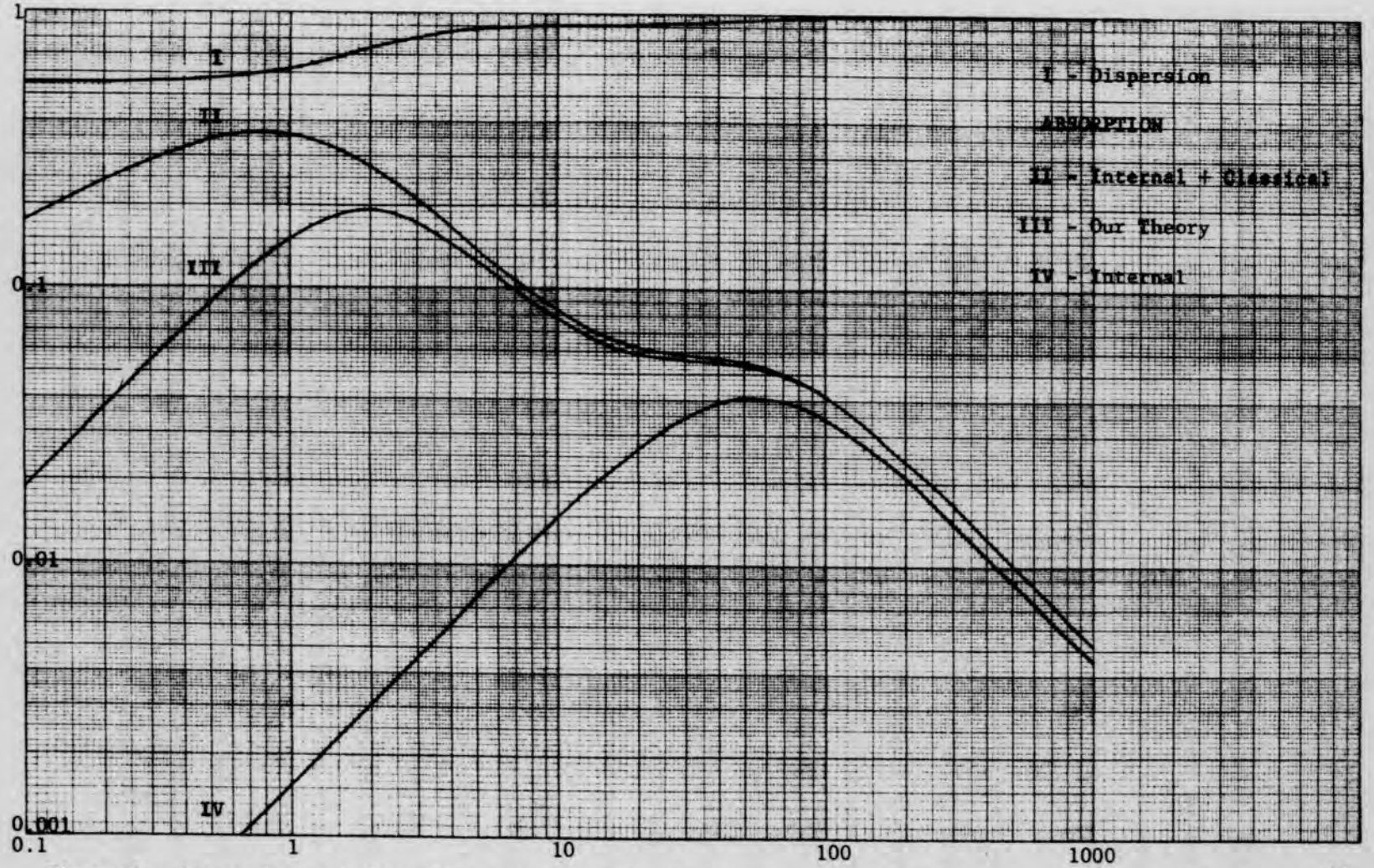

Figure 3. Dispersion and absorption versus the rarefaction parameter for N = 1, h_1 = 1, Z_1 = 100, Z_d = 1

levels off. Our theory exhibits the leveling off equally as well, this corresponding to a greater contribution to the total absorption by the internal (rotational) mode. After $\pi = 100$ our theory and the sum curve again coincide. The dispersion curve approaches unity even more slowly, reaching 0.98 at about $\pi = 100$.

Figure 4 represents the final study of the N = 1 case, where now $Z_1 = 1000$. As is expected, after careful scrutiny of the previous graphs, the internal absorption curve is shifted to the right attaining its greatest value near $\pi = 500$. There is indeed a secondary peak in the sum curve reaching a relative maximum near $\pi = 500$. The relative maximum occurs exactly where anticipated since the greatest contribution by the internal state occurs at this value of π. The curve for our theory exhibits the same shape as does the sum curve; however they coincide only for values of $\pi > 100$. The dispersion has a value of only 0.98 at $\pi = 1000$ indicating that c is still somewhat greater than c_o.

As can be seen from the graphs we have considered, there is a definite relationship between the collision number and the value of π for which the internal absorption curve reaches a maximum. Recalling Eq. (61), let us consider the case for $\pi \ll Z_1$. The fact that $\pi \ll Z_1$ implies that $i\pi Z_1/4\pi \gg 1$ and $h_1/i\pi Z_1/4\pi \approx 0$, meaning that the right-hand side of Eq. (61), is real. Since the negative imaginary part of χ_r is the absorption, it is concluded that $\propto c_o/\omega \approx 0$. For $\pi \gg Z_1$, $i\pi Z_1/4\pi \ll 1$ and the right-hand side of Eq. (61) is again real implying that $\propto c_o/\omega \approx 0$. From computed values only, it appears that the value of π for which the internal absorption is a maximum, is approximately $Z_1/2$.

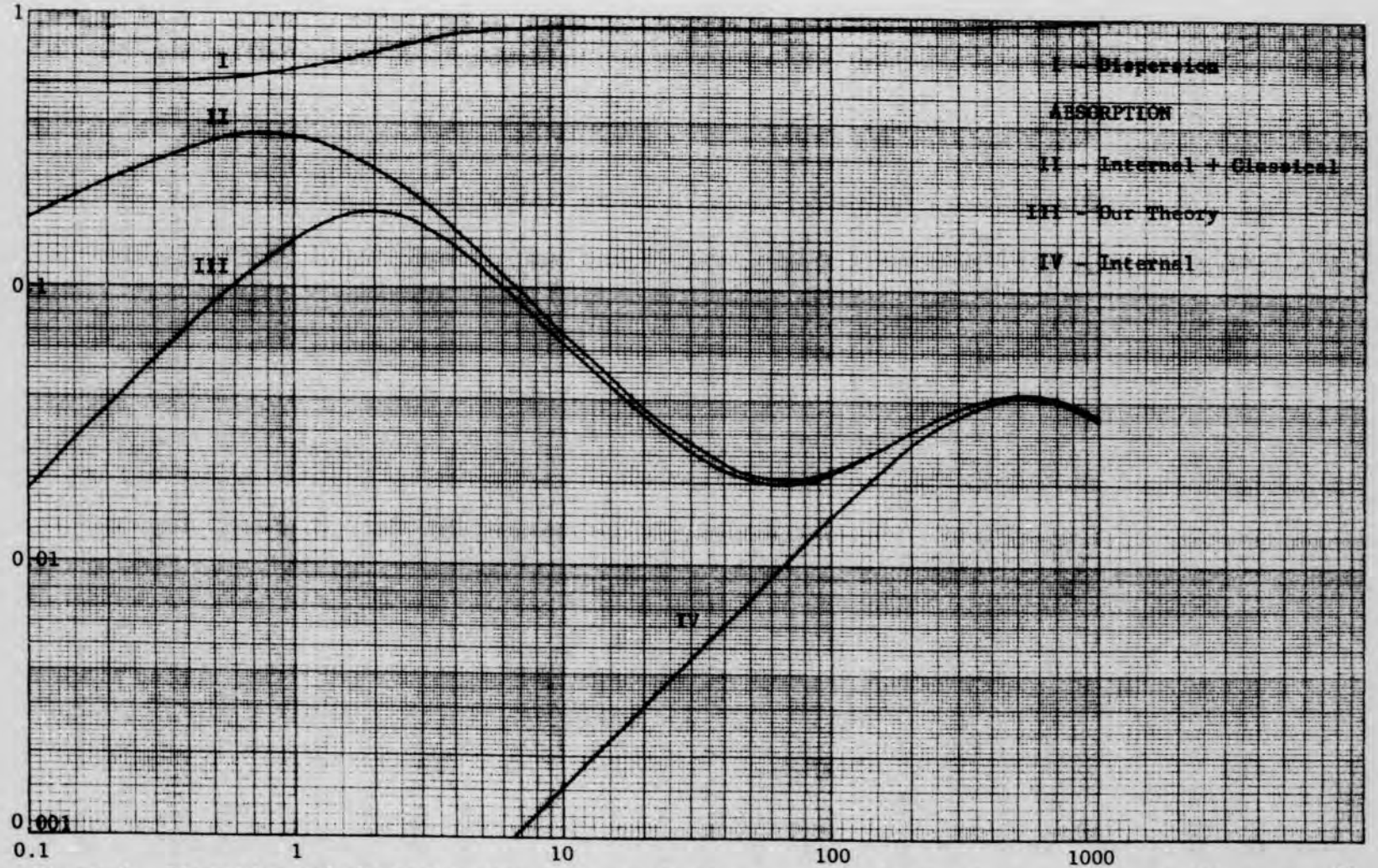

Figure 4. Dispersion and absorption versus the rarefaction parameter for N = 1, h_1 = 1, Z_1 = 1,000, Z_d = 1

If we consider the N = 2 case, we obtain results similar to those discussed above. With two internal modes to consider, the curves for the absorption and dispersion are changed somewhat from the N = 1 case. The quantity Z_1 is the collision number associated with the rotational mode and Z_2 is that for the vibrational mode. For all combinations of the collision numbers considered, $Z_2 > Z_1$, which reflects the experimental fact that most vibrational collision numbers are larger than the rotational collision numbers. It should be noted that for the N = 2 case, we have no comparison criteria as we had before.

In Fig. 5 the effects the rotational and vibrational absorption have on the total absorption are distinctly evident. With $Z_1 = 10$ and $Z_2 = 100$, the absorption due to the rotational and vibrational modes reach maxima near $\Lambda = 5$ and $\Lambda = 50$ respectively. This is evidenced by the fact that there are ever so slight plateau regions near these values of Λ. The dispersion curve is not unlike those investigated previously.

Figure 6 exhibits two distinct plateaus at approximately $\Lambda = 50$ and $\Lambda = 500$. This is exactly what is expected since with $Z_1 = 100$ and $Z_2 = 1000$, we have maxima occuring from the rotational and vibrational absorption near these values of Λ. The dispersion curve rises more gradually than before, which means that the wave is not slowed down as much as it is for $Z_1 = 10$ and $Z_2 = 100$.

For the final pair of collision numbers, $Z_1 = 10$ and $Z_2 = 1000$, there is a secondary peak at about $\Lambda = 500$, as seen in Fig. 7. It is impossible to determine from the absorption curve where the greatest rotational absorption occurs but judging from previous analyses, this

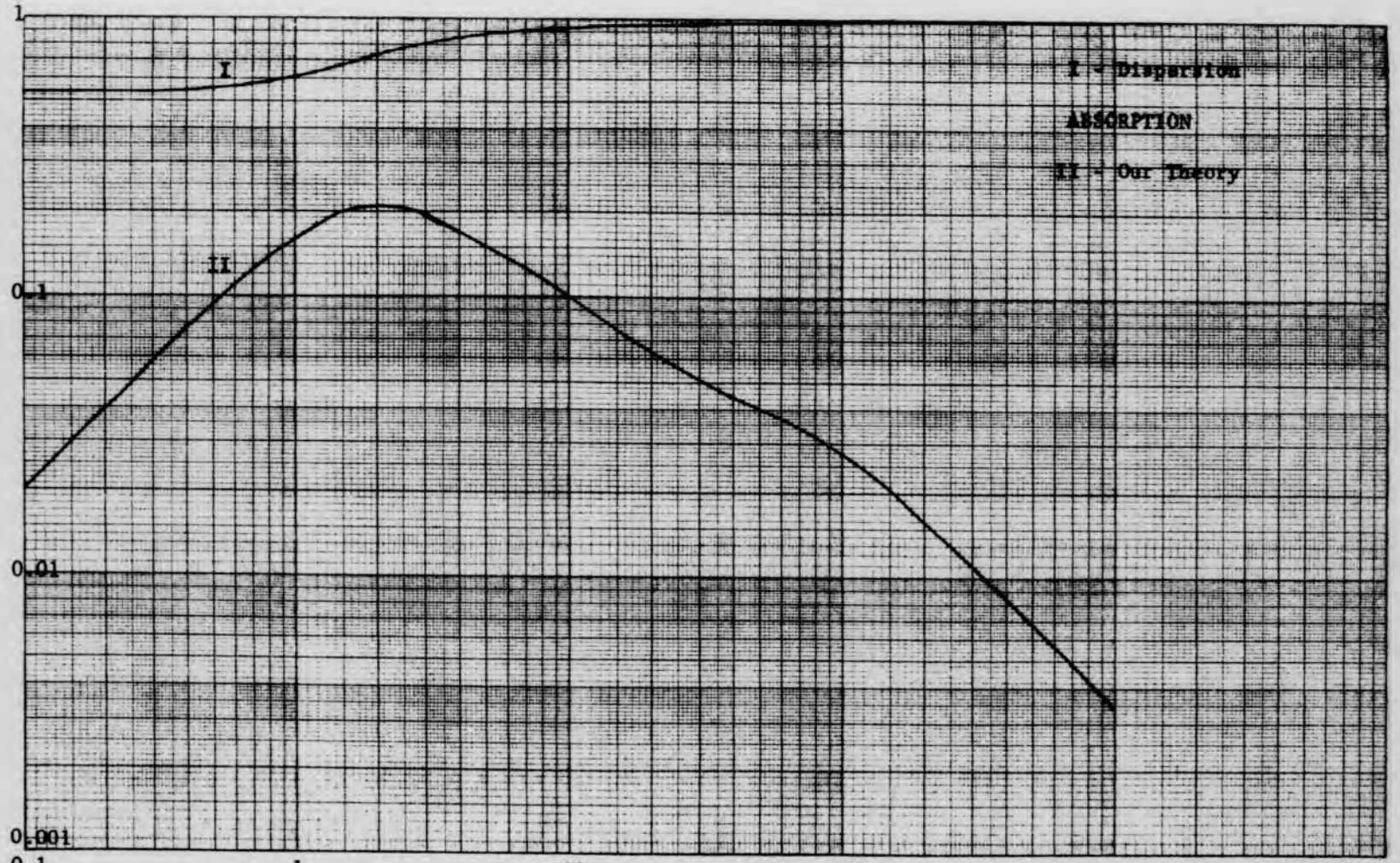

Figure 5. Dispersion and absorption versus the rarefaction parameter for N = 2, h_1 = 1, h_2 = 1, Z_1 = 10, Z_2 = 100, Z_d = 1

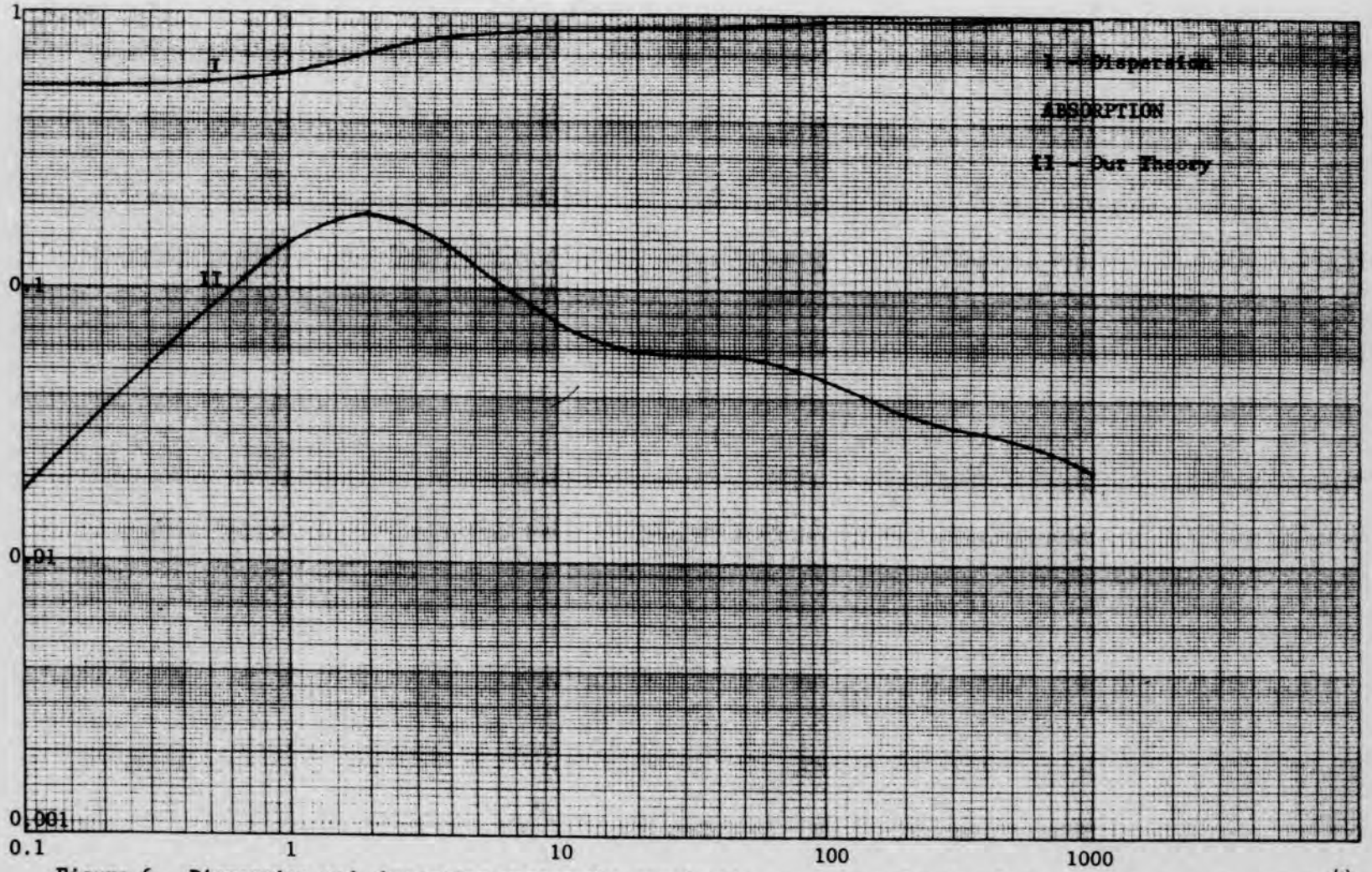

Figure 6. Dispersion and absorption versus the rarefaction parameter for N = 2, h_1 = 1, h_2 = 1, Z_1 = 100, Z_2 = 1000, Z_d = 1

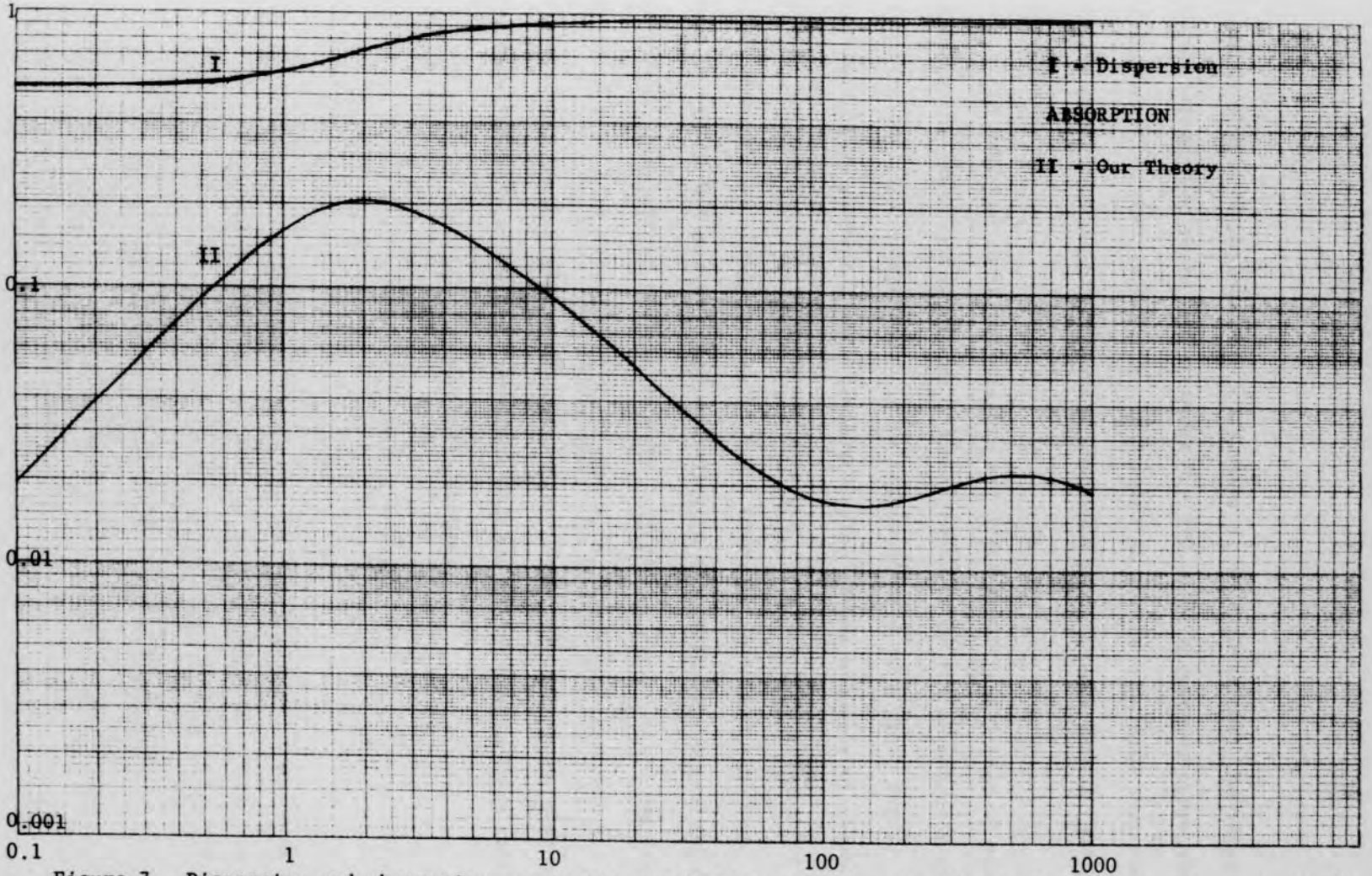

Figure 7. Dispersion and absorption versus the rarefaction parameter for N = 2, h_1 = 1, h_2 = 1, Z_1 = 10, Z_2 = 1000, Z_d = 1

maximum should occur near $\pi = 5$. However it is evident that the vibrational absorption peaks out at about $\pi = 500$. The dispersion curve shows a sharper rise than in Fig. 6 , from which it may be concluded that for larger combined collision numbers, the sound wave travels faster through the medium.

In addition to the absorption and dispersion, recall that we also compute the phase and magnitude of each component of the eigenvector relative to the first component. It is not considered to a great degree informative to present a detailed description of the behavior of these phases and magnitudes. Consequently we give only the general behavior of these quantities. Considering the N = 1 case, all the phases either approach 0° or 90° as $\pi \to \infty$, corresponding to the respective eigenvector component being either real or totally imaginary. The relative magnitudes approach 0 or 1 as $\pi \to \infty$ except X_4/X_1 and X_6/X_1 which both approach $\sqrt{2} - 1$. The case for N = 2 yields similar results. This behavior of the phases and magnitudes obtained from numerical methods agrees exactly with that arrived at by a simplified analytical treatment .

CHAPTER V

CONCLUSIONS

It is reasonable to conclude for the N = 1 case that the theory representing the sum of the classical translational and internal absorptions agrees favorably, for $n > 2$, with the theory we develop for the combined translational and internal absorption. Also it appears that the maximum vibrational and/or rotational contributions to the total absorption occur for values of n of the order of magnitude of the respective collision number. For values of $n << Z_r$ and $n >> Z_r$ the absorption due to the rotational or vibrational modes is neglible. We conclude that for $n << Z_r$ or $n >> Z_r$ the frequency of the wave is so high or so low that neither the rotational nor the vibrational state is capable of exchanging significant amounts of energy with the translational modes. However, for $n \approx Z_r/2$, it appears that the collision frequency of the translational or vibrational mode is in such a relationship with the frequency of the wave itself, that these internal states are capable of exchanging the greatest amounts of energy with the translational states, thereby contributing most to the absorption.

The dispersion of the wave (c_o/c), it should be recalled, is the ratio of the adiabatic speed to the actual sound speed. As alluded to earlier, the rate at which c approaches c_o, decreases as the collision number or numbers increases. The speed c is always greater than c_o but approaches c_o in the low frequency limit, indicating no absorption or impedance of the wave for very low frequencies.

CHAPTER VI

SUMMARY

We have developed a theory, using the 17-moment approximation[1], from which we were able to calculate the absorption and dispersion of sound waves in a general polyatomic gas. This theory proved to be general enough to be valid for many internal degrees of freedom. We limited our study to the case of one internal mode and two internal modes, respectively.

After much arrangement and manipulation we were able to obtain a set of linear equations which were of the form of a general eigenvalue-eigenvector equation. Such an equation was ideal to be solved using computer techniques although we did encounter a few problems with the subroutines until reducing the order of the matrices.

We found that adding the classical translational and internal absorptions analytically gave results which compared favorably, for $N = 1$, with the theory we developed. For $N = 2$, we concluded that our theory was reasonably accurate although we did not have another theory to compare it with.

We observed that the absorption due to internal modes reached a maximum for values of the rarefaction parameter approximately equal to one-half the collision number. Our conclusion was that for these values of π, the frequency of the wave was such that maximum amounts of energy could be exchanged between the translational states and the internal states. Another observation was that, for values of π much greater than or much less than the collision number, the absoption contributed by the internal

states was virtually non-existent. We concluded that, for these corresponding very low frequencies and very high frequencies, there was such a mismatch between the collision frequency and the frequency of the wave that the internal states were not able to exchange significant amounts of energy with the translational states.

As a final analysis of the dispersion of the sound wave, it was observed that for N = 1 the speed of the wave (c) approached the low frequency limit (c_o) much less rapidly as the rotational collision number increased. Similar observations were made for N = 2 where c approached c_o more slowly as the combined rotational and vibrational collision numbers increased.

FOOTNOTES AND BIBLIOGRAPHY

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APPENDIX I

Program Listing

```
//EIGEN JOB ECS.UNCG.PY600048,CREECH T=2,P=60
// EXEC PLC,REGION=225K
//SYSIN DD *
*PLC   (NOATR,NOXREF,TIME=2,PAGES=60)
  EIGEN:PROC OPTIONS(MAIN);
  DCL(IN,N,L,IER) FIXED BINARY;
  GET LIST(IN,N);
  BEGIN;
  DCL(G,AH1,Z1,ZD) BINARY;
  DCL RATIO BIN FLOAT;
  DCL(BETA1,DELTA1,THETA1,THETA2) CPLX BINARY;
  DCL SIGN CHAR(1);
  DCL(SUM,X) CPLX BINARY;  DCL Y BINARY FLOAT;
  DCL((F,AINV)(IN,IN),C(IN,2*IN),B,AB(IN,IN)) CPLX;
  DCL (D,R) BINARY FLOAT;
  DCL(A(N,N),RR(N),RI(N),H(N,N),THETA(7,N),MAGTUD(7,N)) BINARY,
  (CH(N,N),EIG,EV(N,N)) CPLX BINARY,
  (IP(N),I,J,K,M) BINARY FIXED,
  ANA(N) BIT(1);
  DCL (A1(N/2,N/2),EV1(N,N),A1X(N,N),LAMBDX(N,N)) CPLX BINARY;
  DCL Z(7,N) CPLX BINARY;
  LL1: GET LIST(AH1,ZD);
  LL2: GET LIST(Z1);
  DO R=.1 BY .1 TO .9,1 TO 1.8 BY .2,2 TO 3 BY .5,4 TO 9,10 TO 18 BY 2,
 20 TO 30 BY 5,40 TO 90 BY 10,100 TO 180 BY 20,200 TO 300 BY 50,
 400 TO 1000 BY 100;
  G=AH1/Z1;
  THETA2=(3/2-4*G*R/3.14159*1I);
  THETA1=(1-2/3*(1+10/(3*3.14159)*G)*1I*R);
  DELTA1=(1-4*R/(3.14159*Z1)*1I);
  BETA1=(1-2*R/3.14159*(1/ZD+1/Z1)*1I);
  Y=1+1/(1.5+AH1);
  AB(1,1)=1/Y+4/5*1/Y*1/(1-R*1I);
  AB(1,2)=1/Y+8/15*1/Y*1/(1-R*1I)*THETA2;
  AB(1,3)=32/15*1/Y*R/3.14159*AH1/Z1*1I/(1-R*1I);
  AB(2,1)=4/5*1/Y*1/Y*1/(1-R*1I);
  AB(2,2)=1/(Y*Y)*5/2+8/15*1/(Y*Y)*THETA2/(1-R*1I);
  AB(2,3)=32/15*1/(Y*Y)*1/3.14159*AH1/Z1*R*1I/(1-R*1I);
  AB(3,1),AB(3,2)=0; AB(3,3)=AH1/(Y*Y);
  F(1,1)=1;  F(1,2)=0;  F(1,3)=0;
  F(2,1)=-THETA1/Y;
  F(2,2)=THETA1*THETA2/Y-10/3*4/(Z1*Z1)*1/Y*R*R/(3.14159**2)*AH1;
  F(2,3)=R/3.14159*AH1/Z1*(4/Y*THETA1+10/3*1/Y*DELTA1)*1I;
  F(3,1)=-4/3*R/Y*AH1/3.14159*1I/Z1;
  F(3,2)=R/3.14159*AH1/Z1*1I*(4/Y*BETA1+4/3*1/Y*THETA2);
```

```
F(3,3)=DELTA1/Y*AH1*BETA1-16/3*R*R/Y*1/(3.14159**2)*AH1*AH1/(Z1*Z1);
CALL MATINV(IN,F,AINV,IER);
MATINV:PROC (IN,F,AINV,IER);
DCL((F,AINV)(IN,IN),C(IN,2*IN),B) CPLX;
     DO I=1 TO IN;
      DO J=1 TO IN;
      C(I,J)=F(I,J);
     END;
     END;
     L2: DO I=1 TO IN;
     DO J=IN+1 TO 2*IN;
     IF J=IN+I THEN C(I,J)=1;
     ELSE C(I,J)=0;
     END L2;
     L3: DO M=1 TO IN;
     D=ABS(C(M,M));
     DO I=M TO IN;
     IF ABS(C(I,M))>D THEN DO;
     D=ABS(C(I,M));
     L=I;
     END;
     END;
     IF D¬=ABS(C(M,M)) THEN DO;
     DO J=1 TO 2*IN;
     B=C(M,J);
     C(M,J)=C(L,J);
     C(L,J)=B;
     END;
     END;
     B=C(M,M);
IF ABS(B)<0.00001 THEN DO;
      IER=0;
     GO TO L5;
     END;
      ELSE IER=1;
     C(M,*)=C(M,*)/B;
     L4: DO I=1 TO M-1,M+1 TO IN;
     B=C(I,M);
     DO J=M TO 2*IN;
     C(I,J)=C(I,J)-B*C(M,J);
     END;
     END L4;
     END L3;
     DO J=IN+1 TO 2*IN;
     AINV(*,J-IN)=C(*,J);
      END;
     L5:END MATINV;
DO I=1 TO N/2;
DO J=1 TO N/2;
SUM=0;
DO K=1 TO N/2;
```

```
SUM=SUM+AINV(I,K)*AB(K,J);
END;
A1(I,J)=SUM;
END;
END;
DO I=1 TO N;
DO J=1 TO N;
IF I<=N/2&J<=N/2 THEN A(I,J)=REAL(A1(I,J));
IF I>N/2&J>N/2 THEN A(I,J)=REAL(A1(I-N/2,J-N/2));
IF I<=N/2&J>N/2 THEN A(I,J)=-IMAG(A1(I,J-N/2));
IF I>N/2&J<=N/2 THEN A(I,J)=IMAG(A1(I-N/2,J));
END;
END;
CALL MATE(A,N,IP);
H=A;
CALL MEAT(A,N,RR,RI,ANA);
I=0;
DO M=1 TO N;
I=I+1;
EIG=COMPLEX(RR(M),RI(M));
CH(1,*)=H(1,*);
DO J=2 TO N;
DO K=J-1 TO N;
CH(J,K)=H(J,K);
END;
END;
CALL MVAT(CH,N,EIG,EV(*,I));
CALL MVEB(H,N,IP,EV(*,I));
DO J=1 TO N/2;
EV1(J,I)=EV(J,I); END;
DO J=1 TO N/2;
SUM=0;
DO K=1 TO N/2;
SUM=SUM+A1(J,K)*EV1(K,I);
END;
A1X(J,I)=SUM;
LAMBDX(J,I)=EIG*EV1(J,I);
END;
L=0;
DO J=1 TO N/2;
IF ABS(LAMBDX(J,I)-A1X(J,I))<0.00001 THEN L=L+1;
END;
IF ABS(L-N/2)<0.01 THEN DO;
X=1/(SQRT(EIG));
PUT SKIP;
PUT DATA(X,Z1);
Z(1,I)=EV(1,I); Z(4,I)=EV(2,I); Z(6,I)=EV(3,I);
Z(3,I)=8/15*THETA2*1/Y*Z(4,I)/(1-R*1I)+8/15*3/(2*Y)*Z(1,I)/(1-R*1I)+
8/15*1I/3.14159*4/Y*AH1/Z1*R*Z(6,I)/(1-R*1I);
```

```
   IF REAL(X)>0&IMAG(X)<0 THEN DO;
   Z(2,I)=Z(1,I)*SQRT(EIG);
   Z(5,I)=(15/8*(1-R*1I)*Z(3,I)-5/2*Z(1,I)/Y)*SQRT(EIG);
   Z(7,I)=(DELTA1*1/Y*AH1*Z(6,I)+4/3.14159*1I/Y*AH1/Z1*R*Z(4,I))*
  SQRT(EIG);
   END;
   ELSE DO;
   Z(2,I)=Z(1,I)*(-SQRT(EIG));
   Z(5,I)=(15/8*(1-R*1I)*Z(3,I)-5/2*Z(1,I)/Y)*(-SQRT(EIG));
   Z(7,I)=(DELTA1*1/Y*AH1*Z(6,I)+4/3.14159*1I/Y*AH1/Z1*R*Z(4,I))*
  (-SQRT(EIG));
   END;
   RATIO=1/REAL(X)-1;  PUT DATA(RATIO);
   PUT SKIP EDIT(R,ABS(IMAG(X)),REAL(X))(F(10,5),X(5),F(10,5),X(4),F(
  10,5));
   DO J=1 TO N+1;
   IF IMAG(Z(J,I))<0 THEN SIGN='-';
   ELSE SIGN='+';
   T1=REAL(Z(J,I));  T2=IMAG(Z(J,I));
   T3=REAL(Z(1,I)); T4=IMAG(Z(1,I));
  IF IMAG(Z(J,I))=0 & REAL(Z(J,I))=0 THEN THETA(J,I)=0;
   ELSE THETA(J,I)=ATAND(T2,T1)-ATAND(T4,T3);
   IF ABS(IMAG(Z(1,I)))<0.0001&ABS(REAL(Z(1,I)))<0.0001 THEN MAGTUD(J,I)
  =0;
   ELSE MAGTUD(J,I)=ABS(Z(J,I))/ABS(Z(1,I));
   PUT EDIT(REAL(Z(J,I)),SIGN,ABS(IMAG(Z(J,I))),'I',THETA(J,I),MAGTUD(J,I
  ))(COLUMN(43), 2(F(10,5),A),X(5),F(10,5),X(11),F(10,5),SKIP);
   END;
   PUT SKIP;
   END;
   GO TO LL3;
   END;
   LL3: END;
   GO TO LL2;
   END;
   END EIGEN;
*DATA
3,6
1.0,1.0,1.0,10,100,1000
/*
//
```